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NUCLEIC ACID SEQUENCES CODING
FOR PROTEINS OF UNKNOWN
STRUCTURE AND FUNCTION

PARSE DISEASE GENES INTO
DOMAIN-ENCODING REGIONS

DOMAIN TRAPPING: EXPRESSION &
BIOPHYSICAL CHARACTERIZATION

HIGH YIELD EXPRESSION, ISOTOPE
ENRICHMENT, & PURIFICATION

SCREENING FOR NMR &
CRYSTALLIZATION PROPERTIES

ANALYSIS OF PROTEIN STRUCTURE
BY NMR & X-RAYS

TERTIARY STRUCTURE HOMOLOGY
SEARCH OF PROTEIN DATA BASE

STRUCTURE/FUNCTION
KNOWLEDGE BASE

ASSIGNMENT OF DOMAIN TO
FOLD & FUNCTIONAL CLASS

KNOWLEDGE-
BASED PARSING
METHOD

DATABASE
OF EMPIRICAL
PROPERTIES

RELATIONAL
DATABASE

FIG.1

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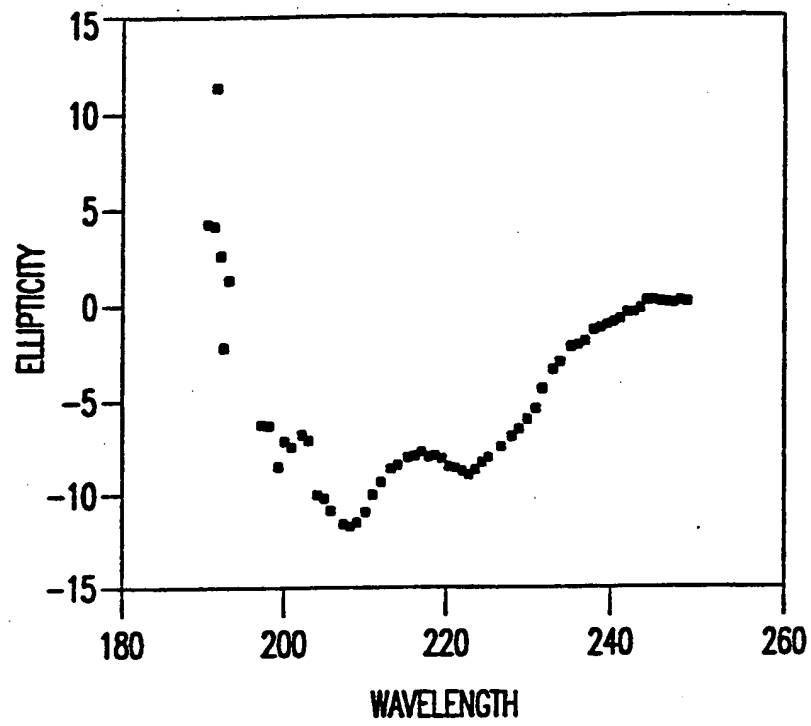


FIG. 2A

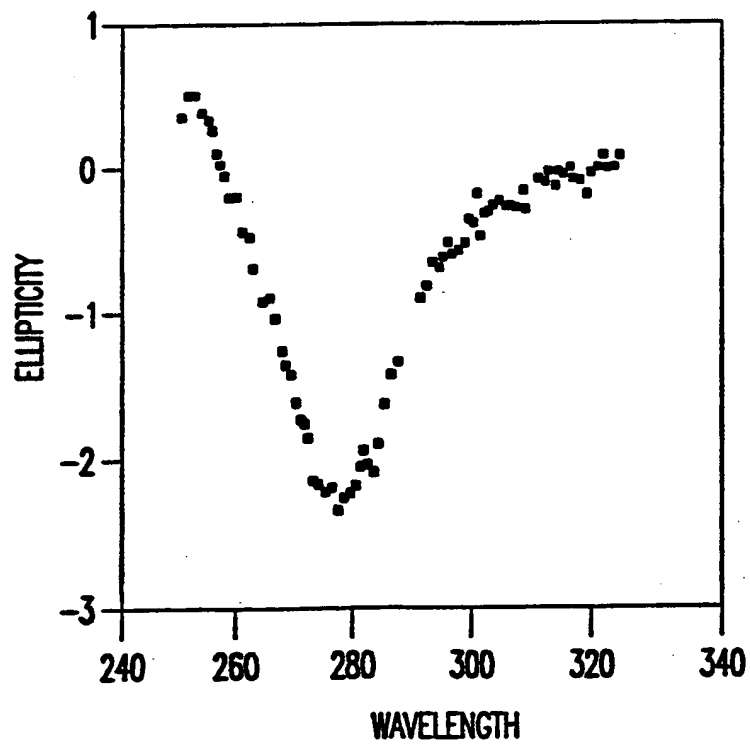


FIG. 2B

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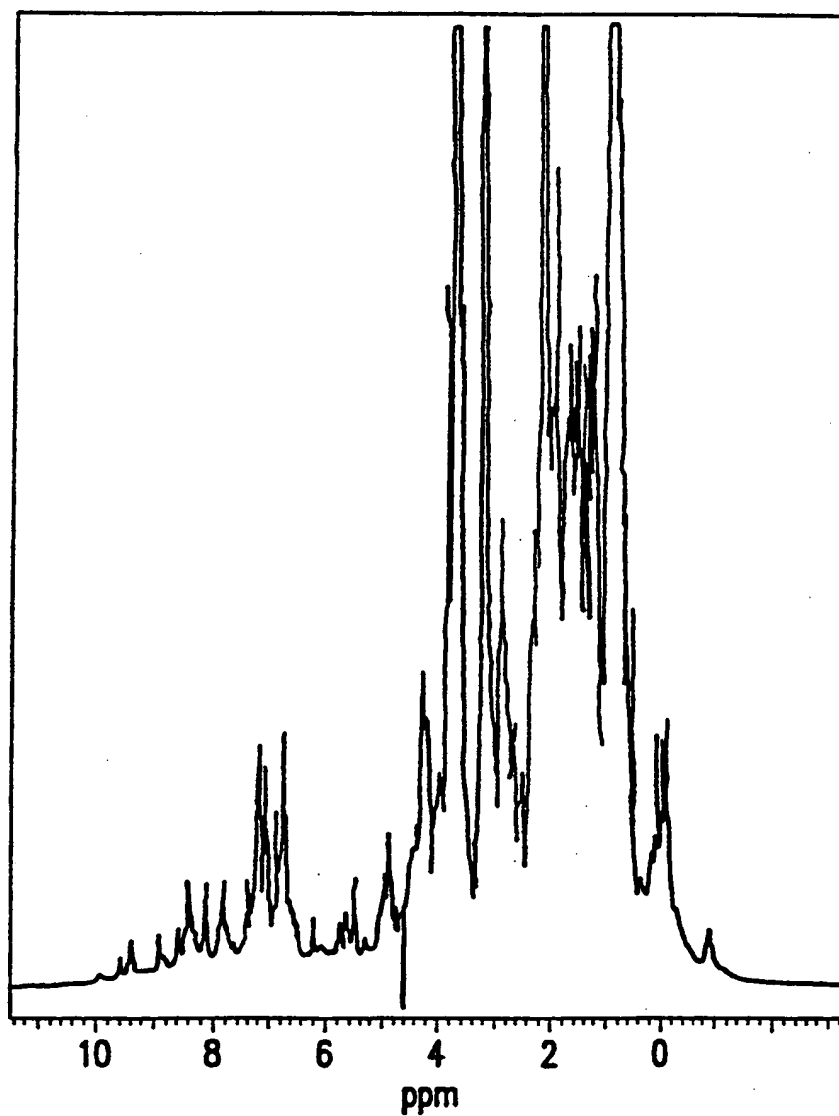


FIG.3

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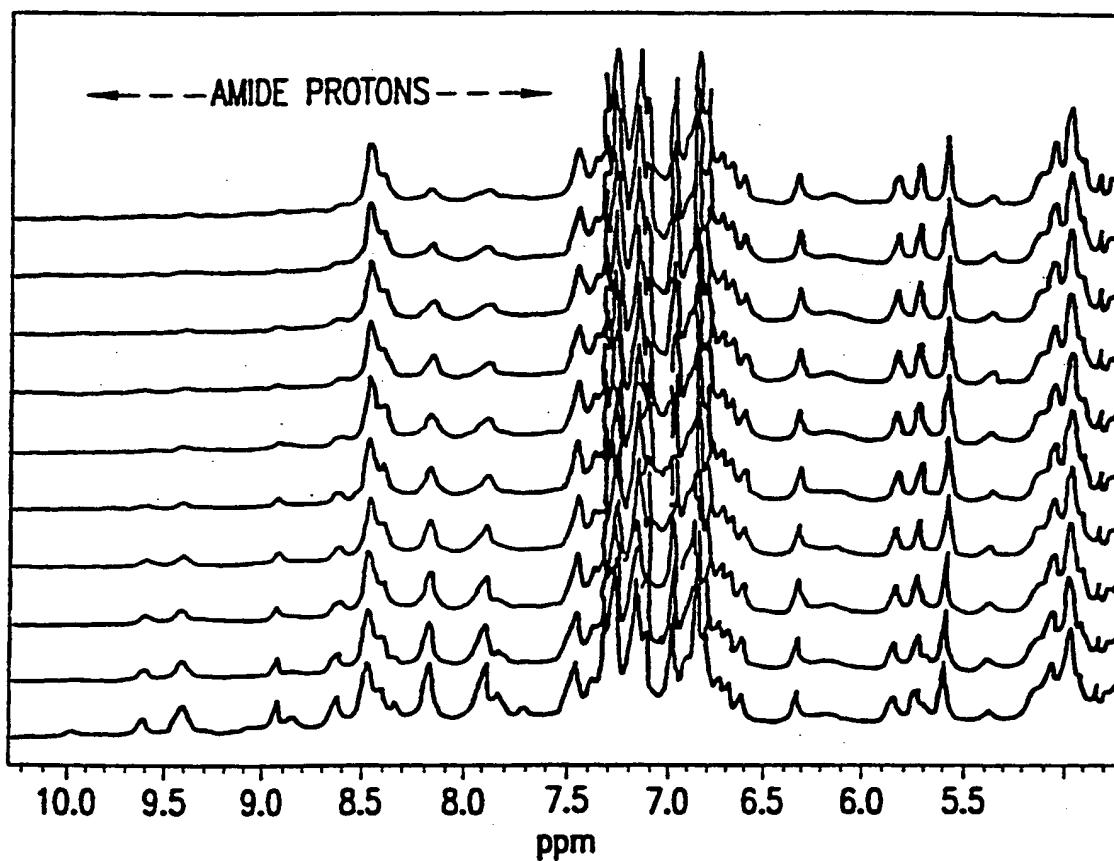


FIG.4

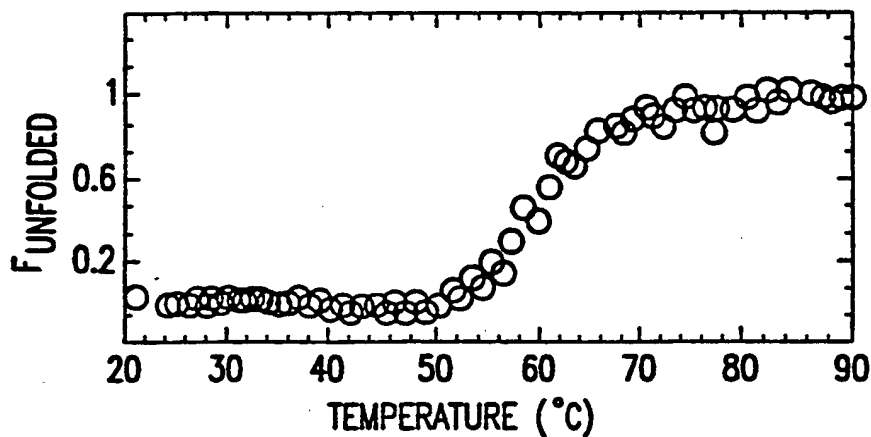
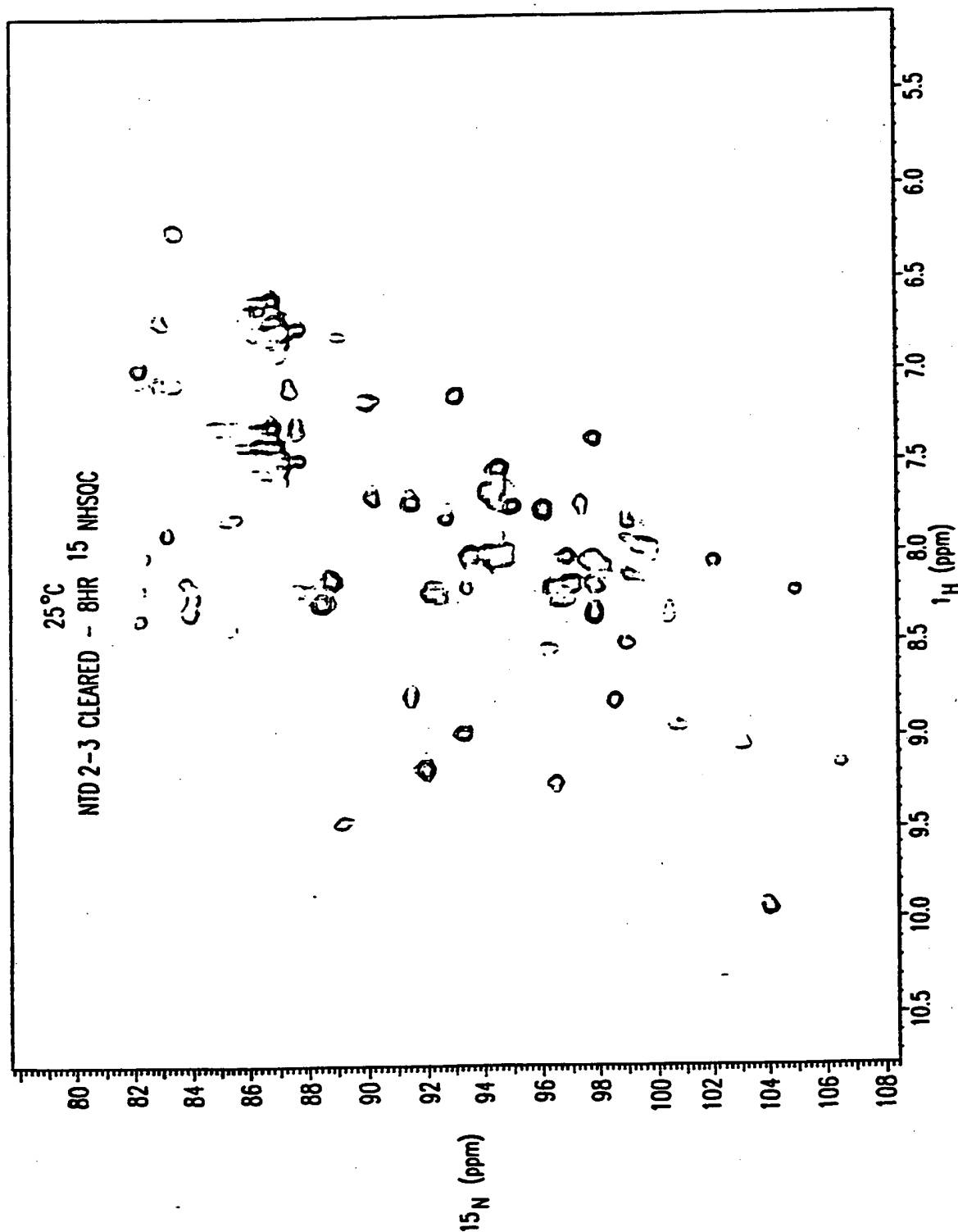


FIG.5

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FIG. 6



102080" 20044460

WO 00/05

09/744002

PCT/US99/16417

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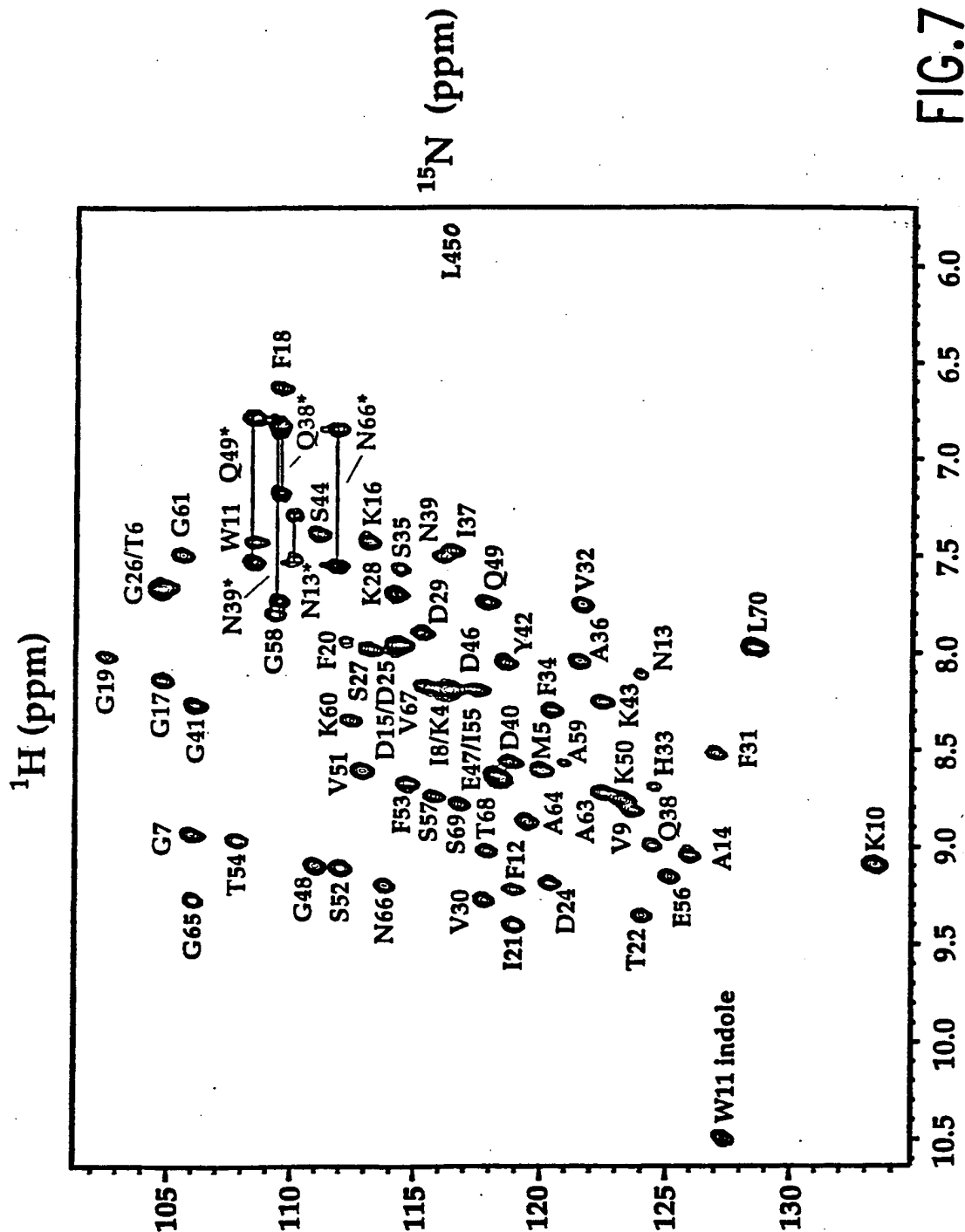


FIG. 7

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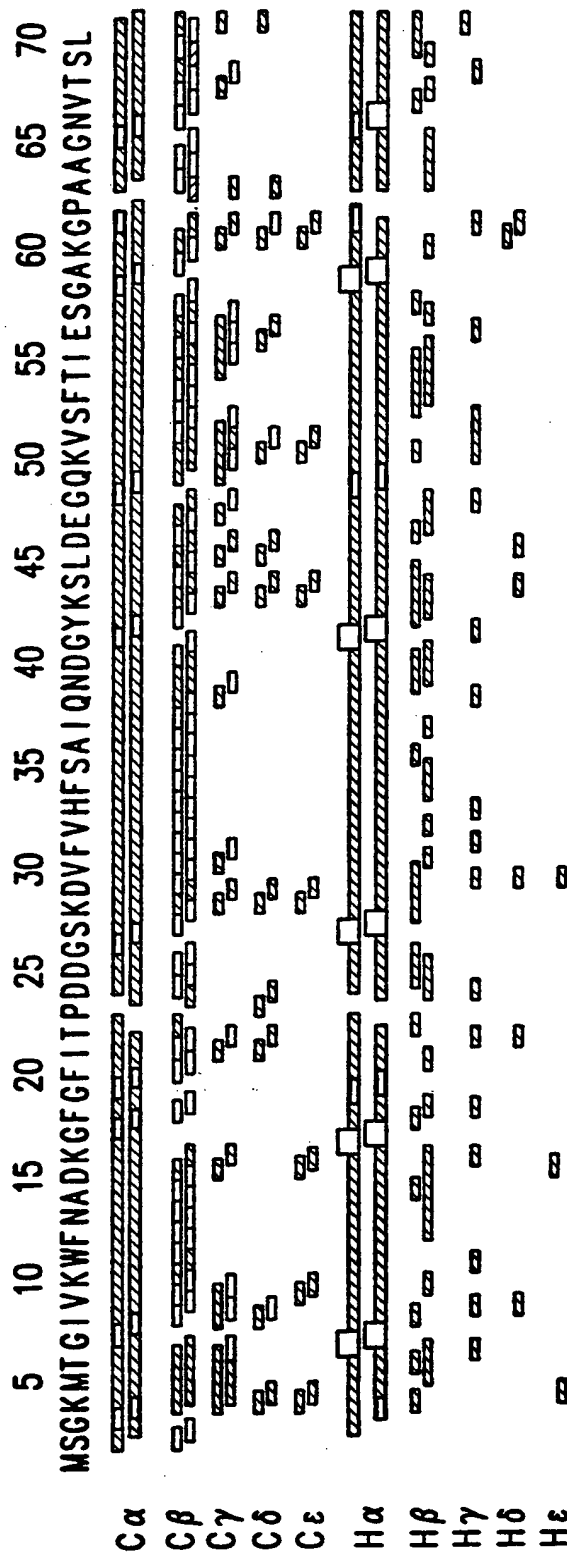


FIG.8A



FIG. 8B

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NOESY_ASSIGN PROCESS

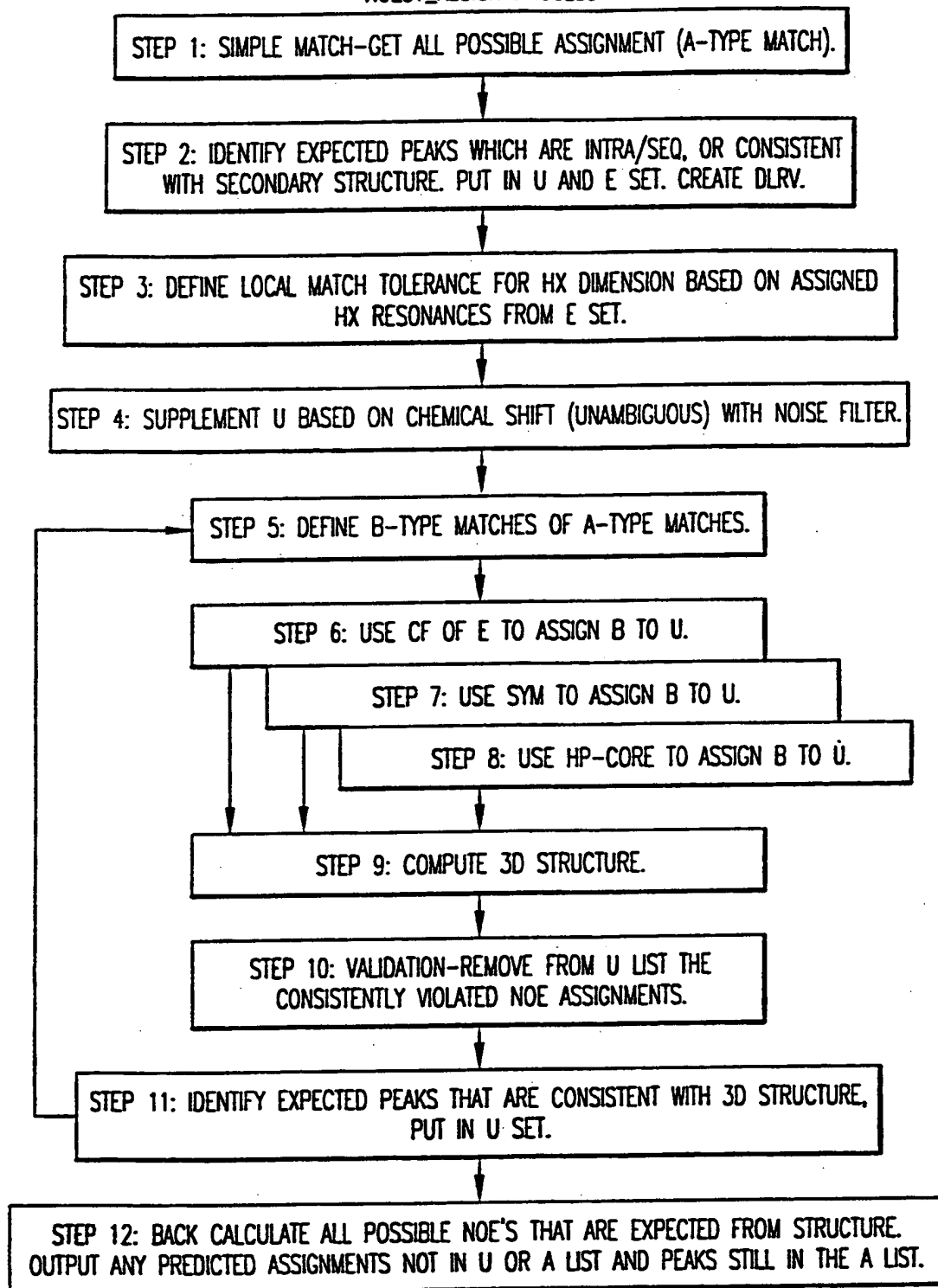
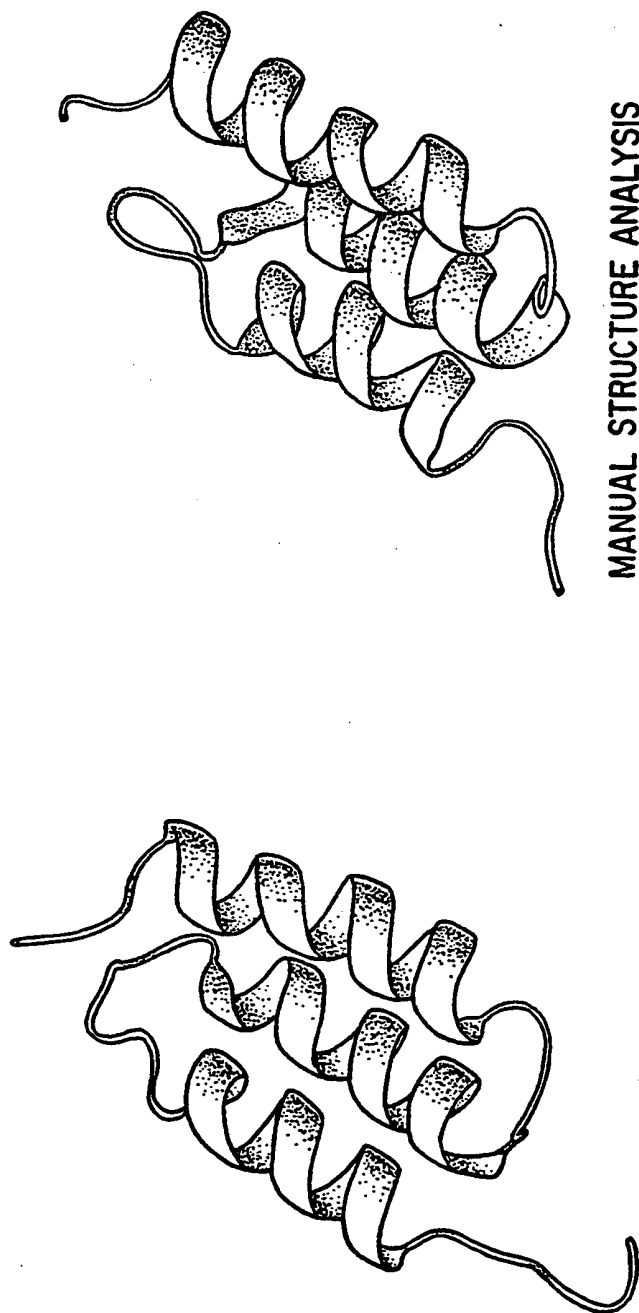


FIG.9

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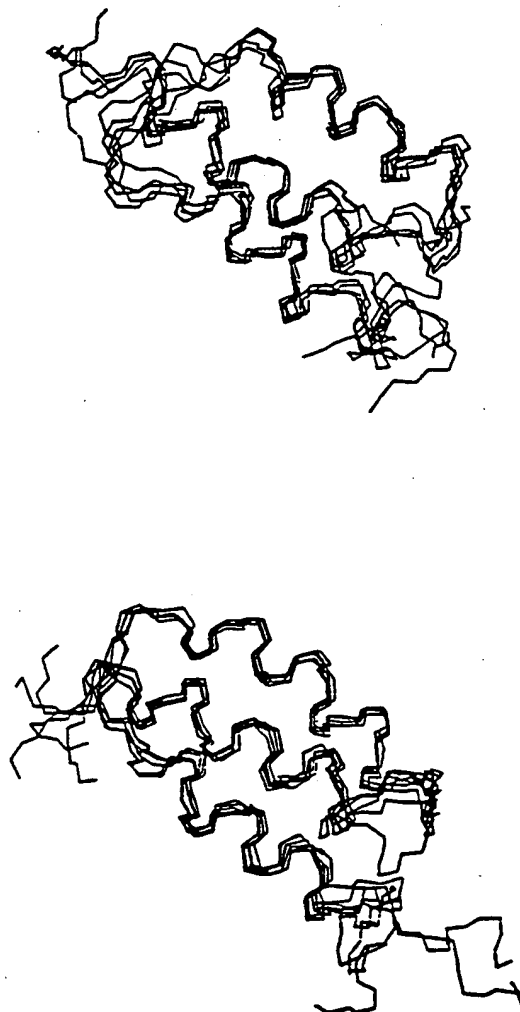


MANUAL STRUCTURE ANALYSIS

AUTOMATED STRUCTURE ANALYSIS

FIG.10A

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Automated Structure Analysis Manual Structure Analysis

FIG.10B

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Zdom: Automated Assignment Analysis

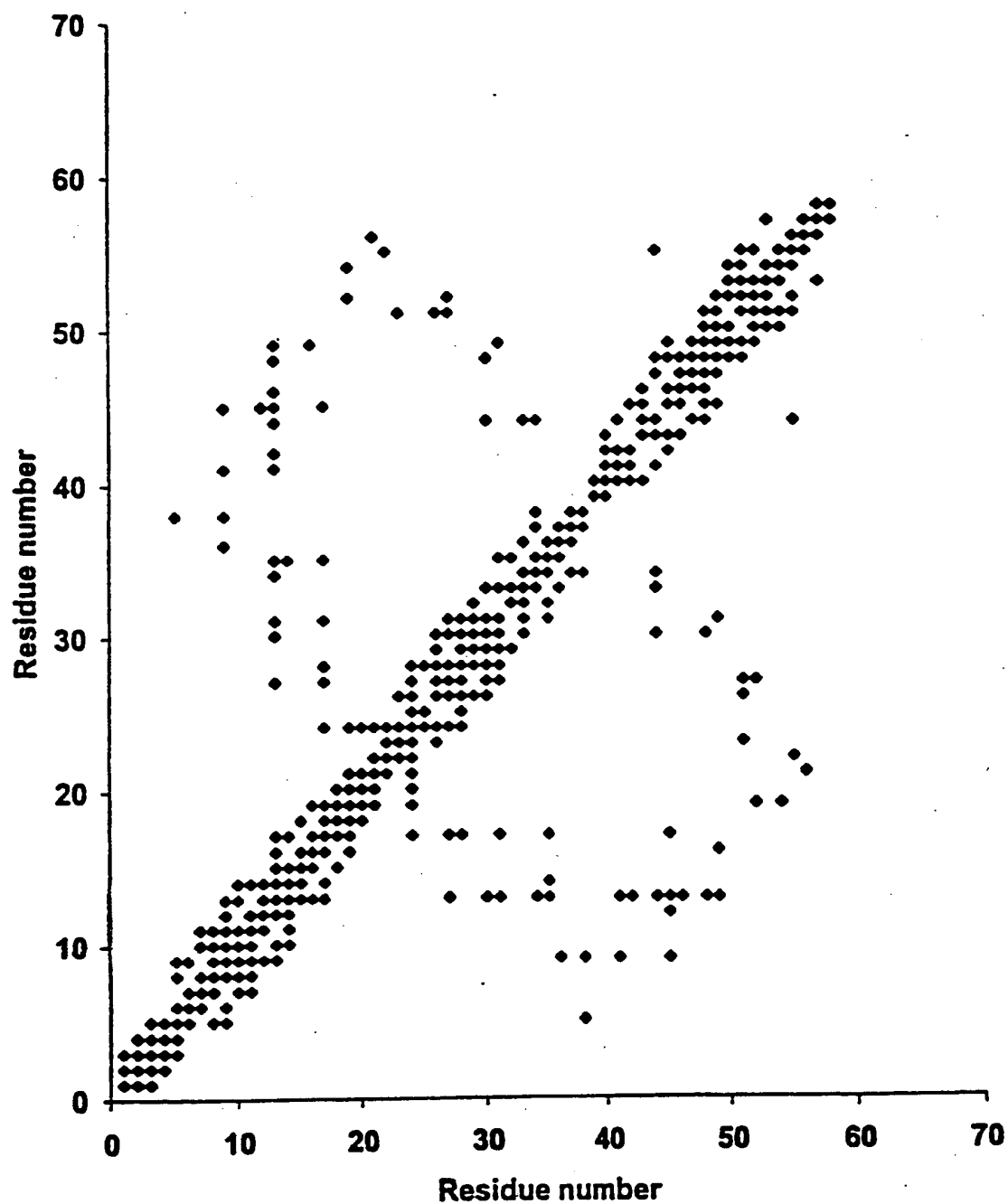


FIG.11

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Zdom: AUTOMATED STRUCTURE ANALYSIS

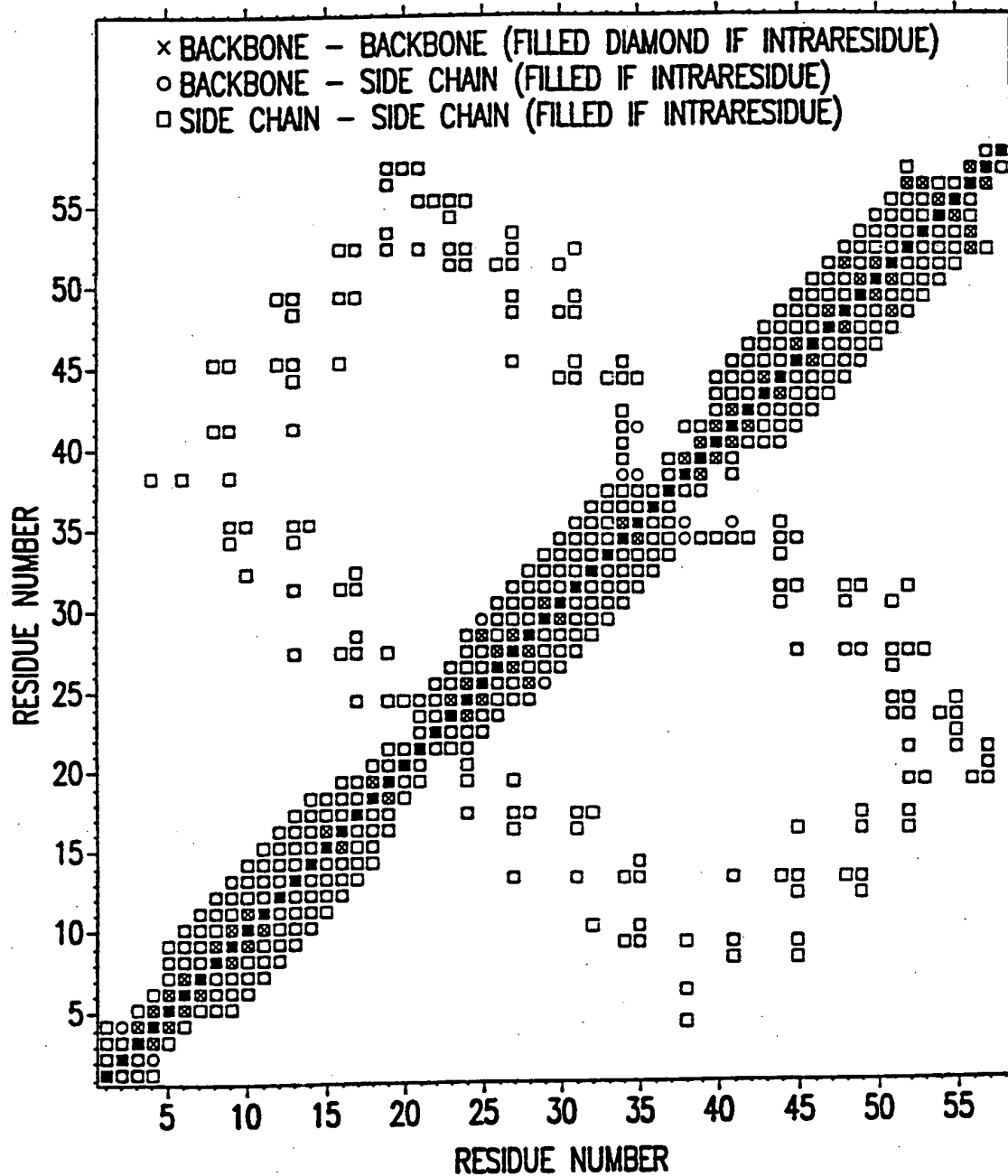


FIG.12

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Zdom: AUTOMATED ANALYSIS-CONNECTIVITY MAP

0 1 2 3
0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0

$NN(i,i+1)$ —————
 $\alpha N(i,i+1)$ —————
 $\alpha N(i,i+3)$ —————
 $\alpha \beta(i,i+3)$ —————

3 4 5 6
0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0

$NN(i,i+1)$ —————
 $\alpha N(i,i+1)$ —————
 $\alpha N(i,i+3)$ —————
 $\alpha \beta(i,i+3)$ —————

FIG.13

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Zdom: Manual Assignment Analysis

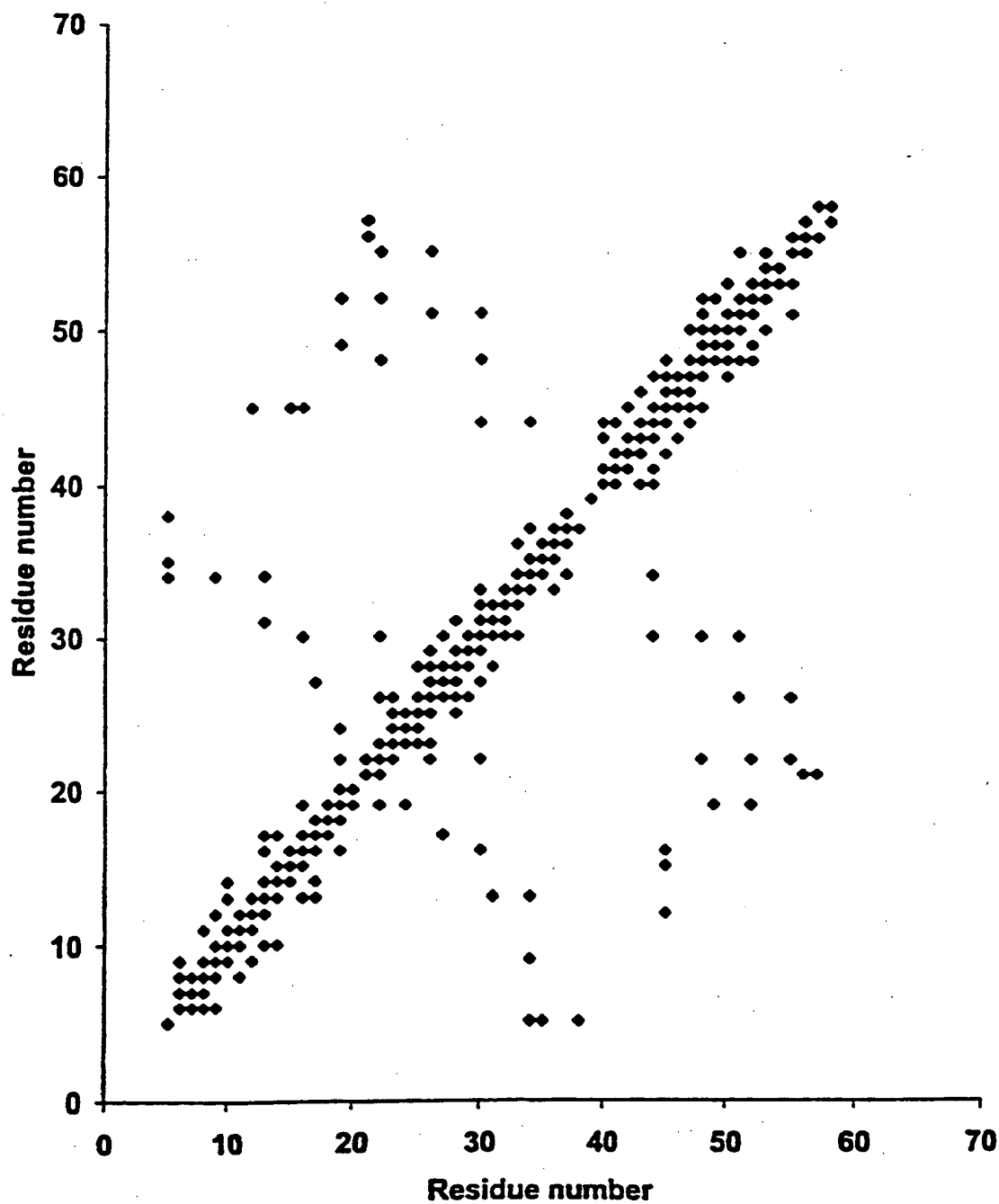


FIG.14

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Zdom: MANUAL STRUCTURE ANALYSIS

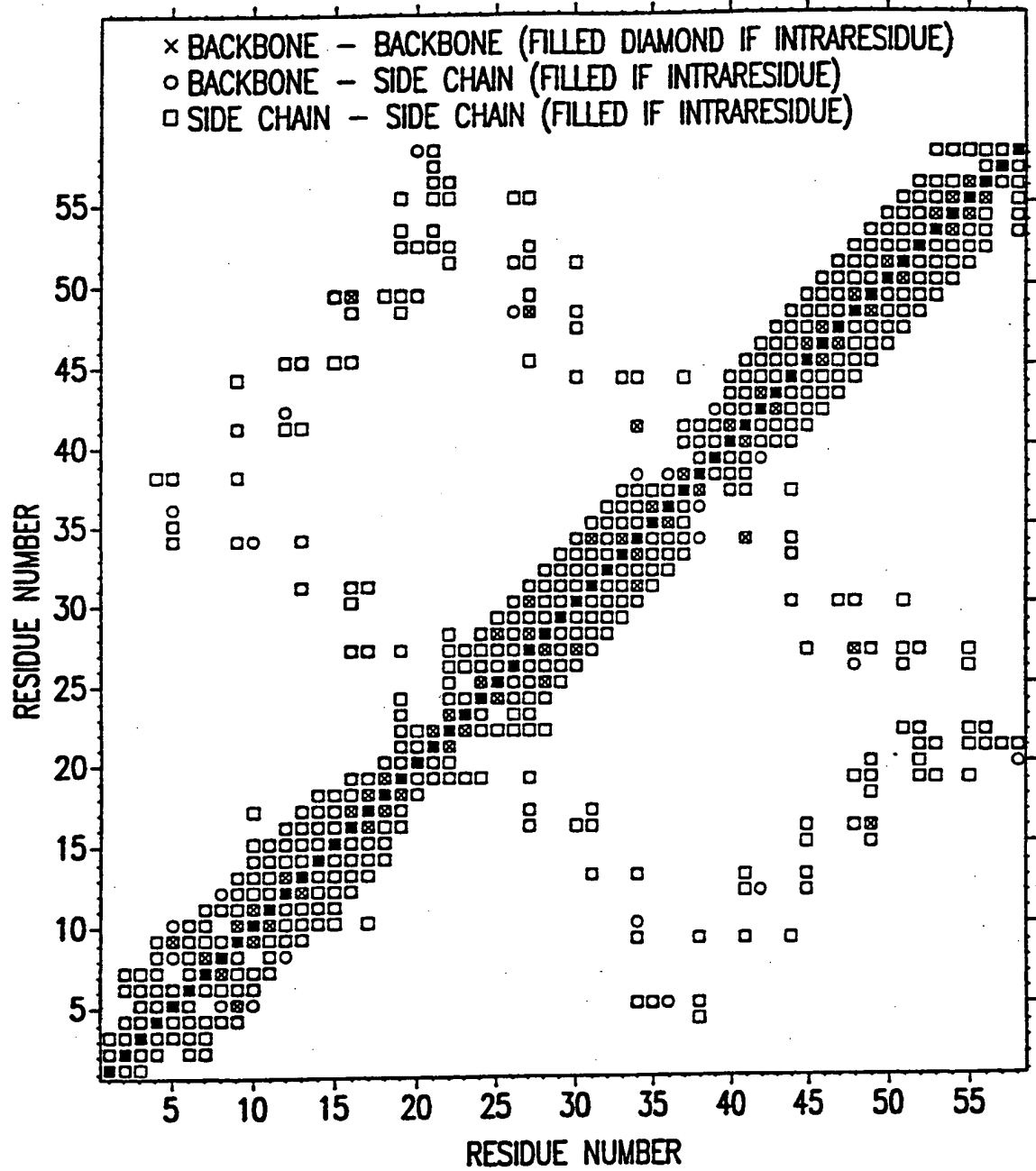


FIG.15

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Zdom: AUTOMATED ANALYSIS-CONNECTIVITY MAP

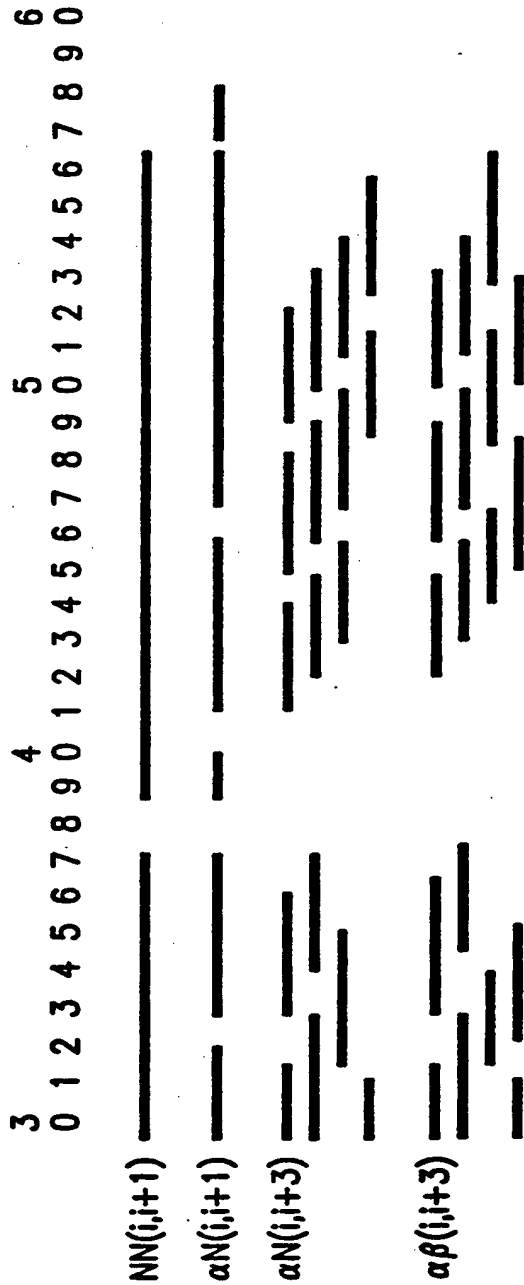
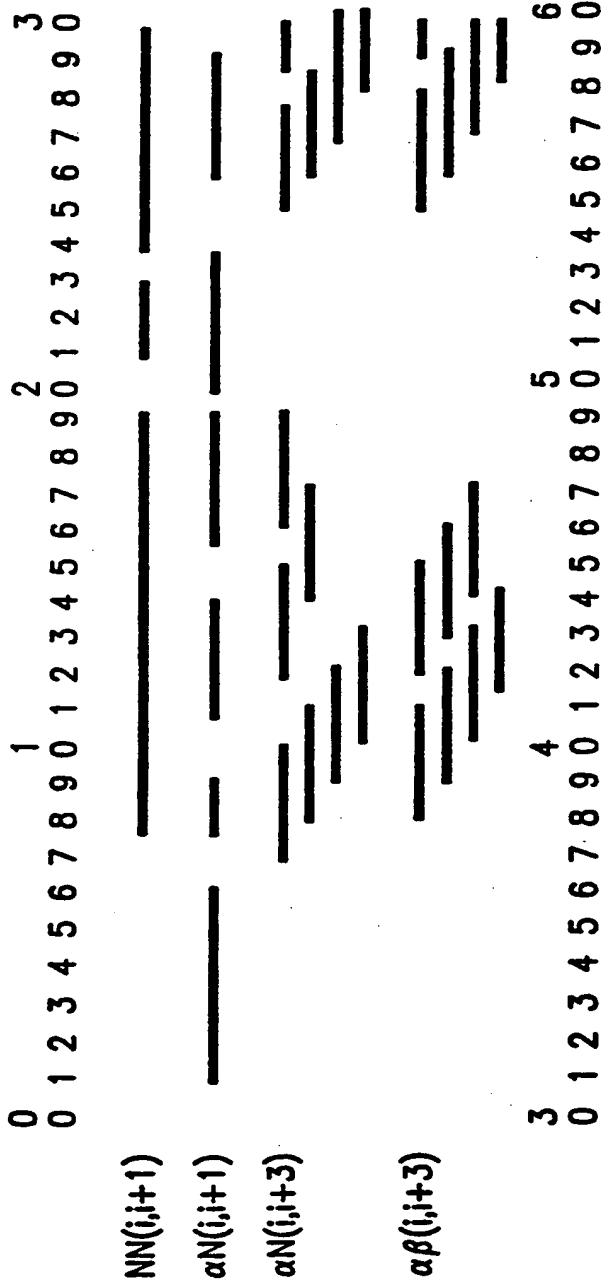
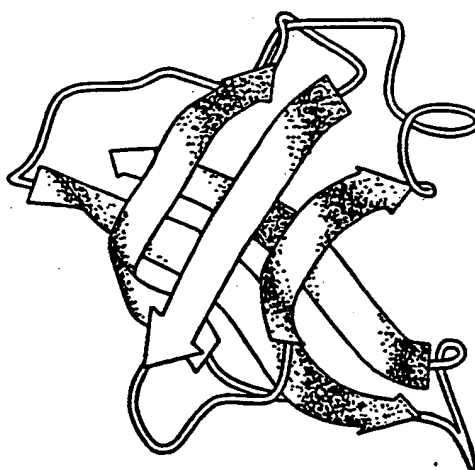


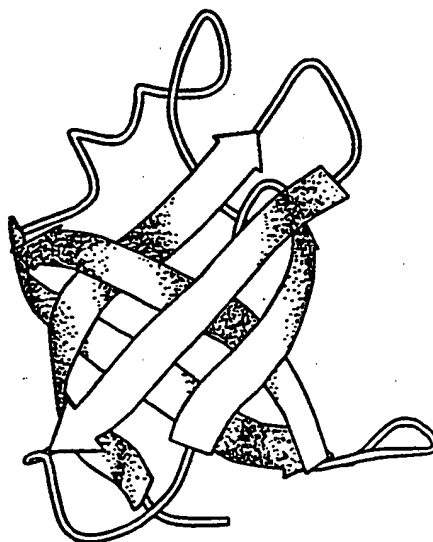
FIG.16

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CspA



AUTOMATED STRUCTURE ANALYSIS



MANUAL STRUCTURE ANALYSIS

FIG.17

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Cspa: Automated Assignment Analysis

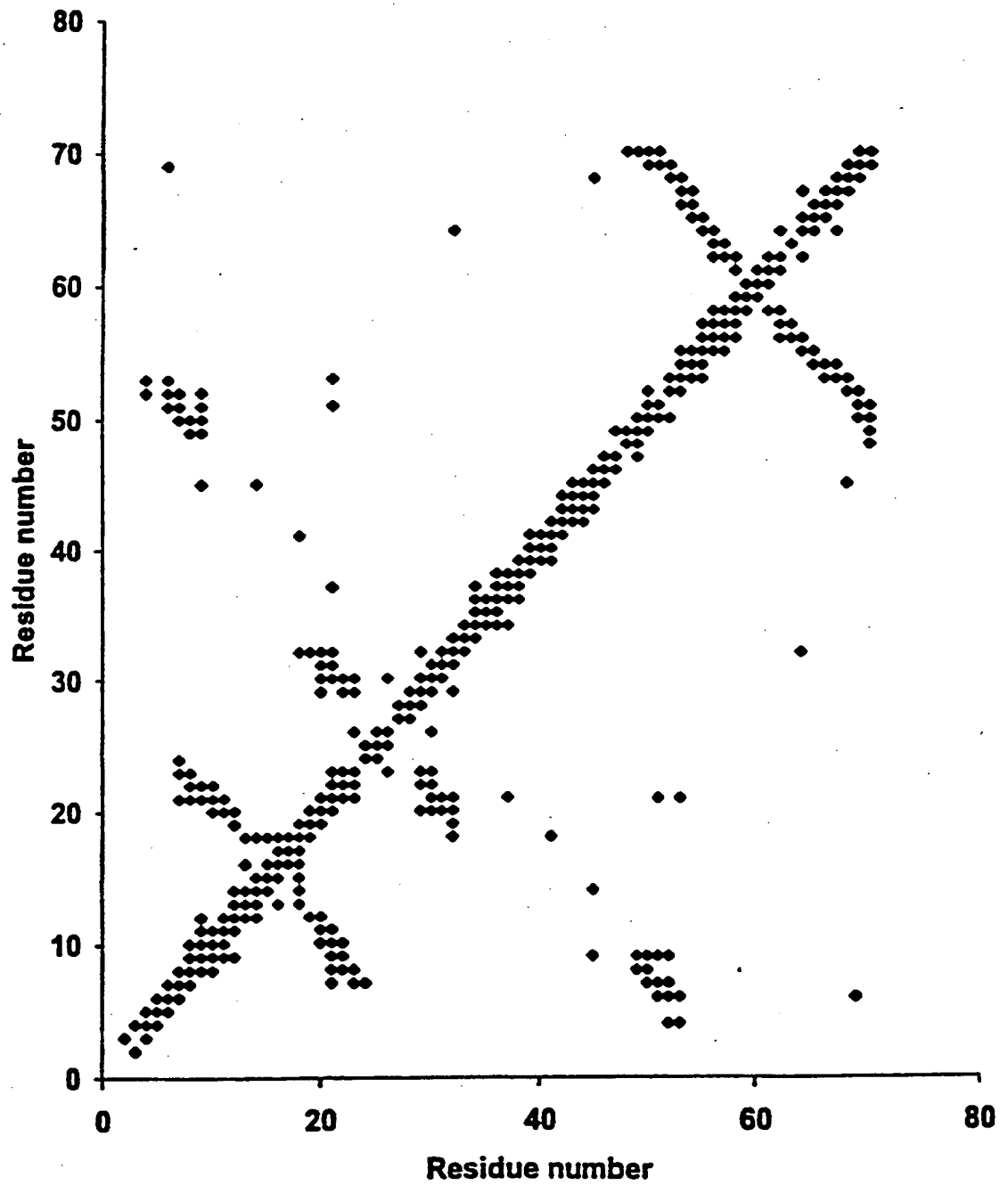


FIG.18

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Cspa: AUTOMATED STRUCTURE ANALYSIS

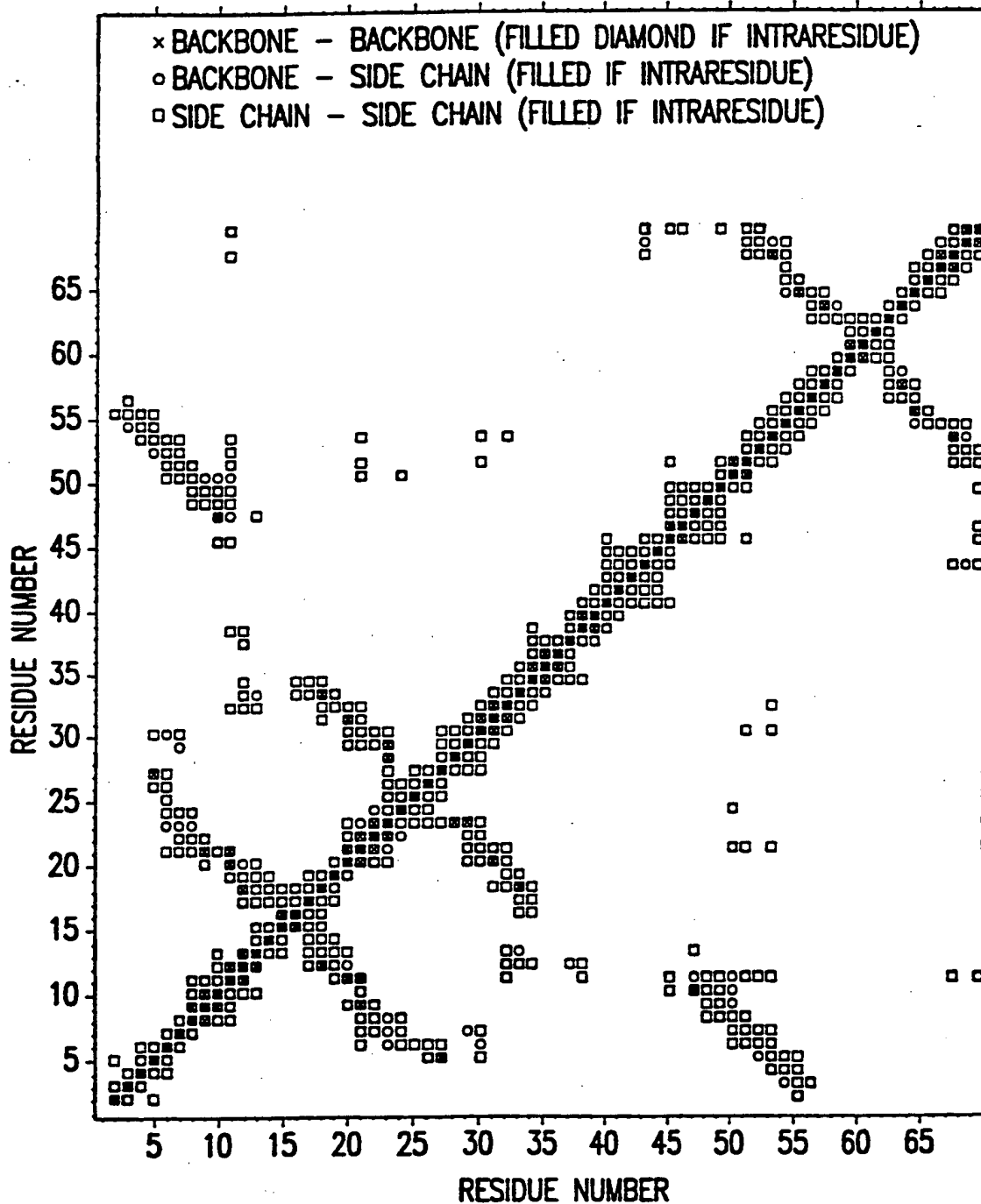


FIG.19

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Cspa: AUTOMATED ANALYSIS--CONNECTIVITY MAP

[illegible]

$NN(i,i+1)$	—	—	—	—	—
$\alpha N(i,i+1)$	—	—	—	—	—
$\alpha N(i,i+3)$	—	—	—	—	—

[illegible]

FIG. 20

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Cspa: Manual Assignment Analysis

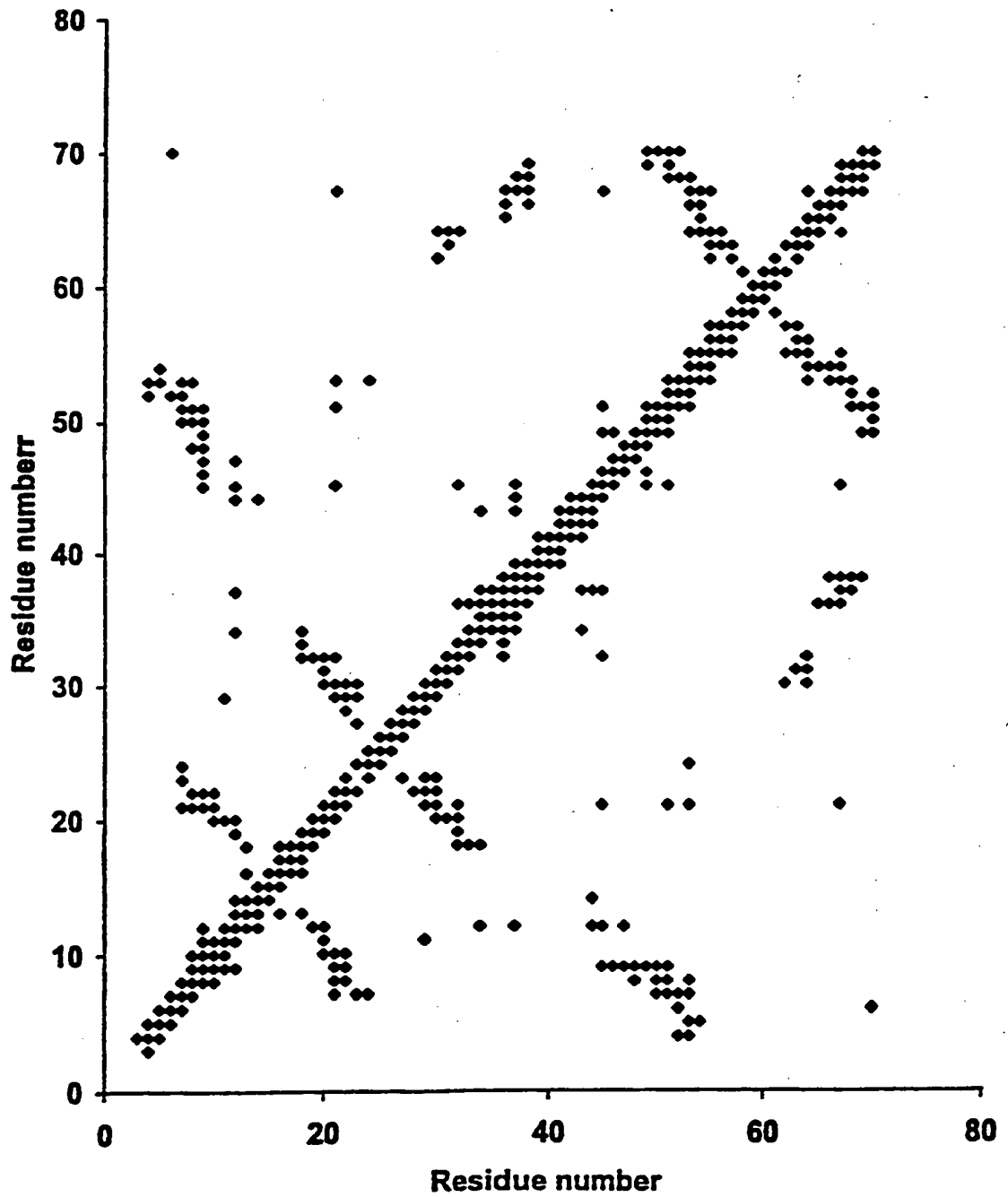


FIG.21

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Cspa: MANUAL STRUCTURE ANALYSIS

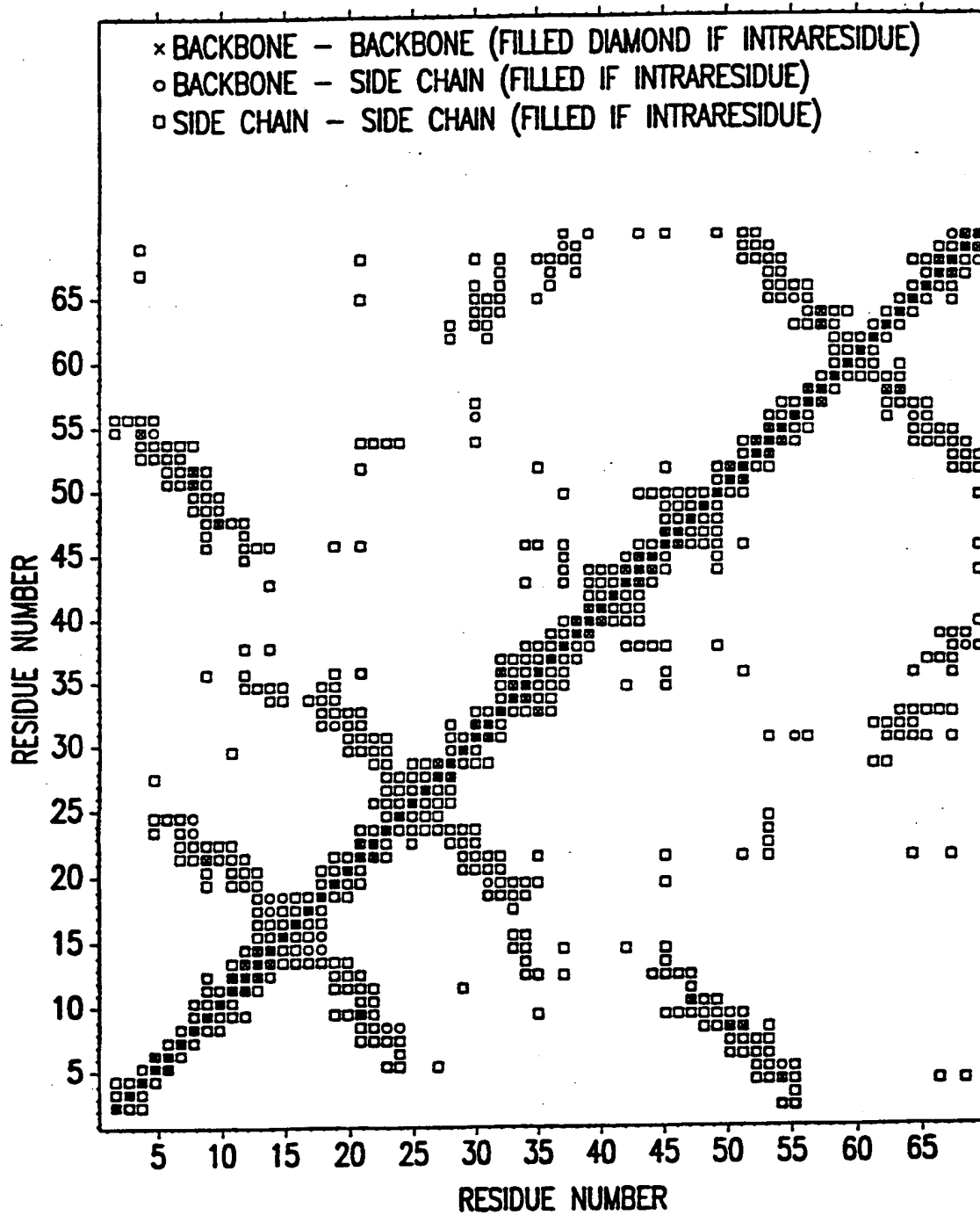


FIG.22

Cspa: MANUAL ANALYSIS--CONNECTIVITY MAP

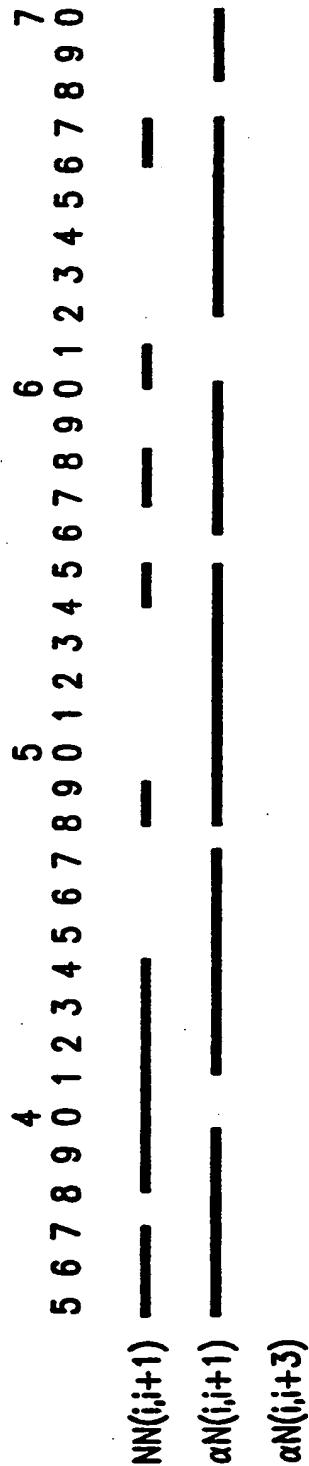
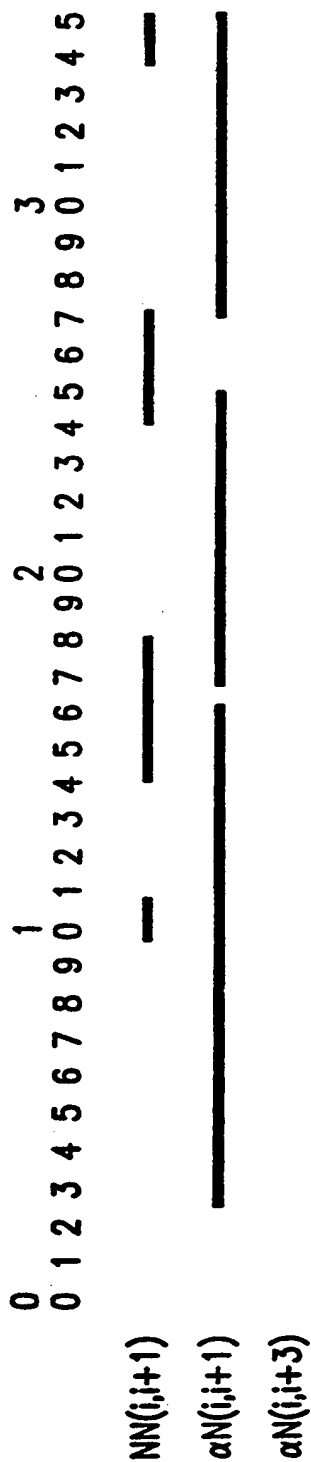


FIG.23